

A simple regression equivalence of Pillai's trace statistic

BY XIA SHEN, ZHENG NING, YUDI PAWITAN

*Department of Medical Epidemiology and Biostatistics, Karolinska Institutet
SE-17 177 Stockholm, Sweden*

Consider Pillai's trace $V^{(1)}$ statistic (denoted as V hereafter) [Pillai, 1955] for a multivariate analysis of variance (MANOVA) problem with an independent variable $x_{n \times 1}$ and multiple dependent variables $Y_{n \times k}$, where Y is column-full-ranked. Let us reverse the problem as a linear multiple regression

$$x = a1 + Yb + e. \quad (1)$$

Let $\hat{b} = (Y^T Y)^{-1} Y^T x$ be the least-squares estimate of b . Define a score $s_{n \times 1} = Y\hat{b}$ as a linear combination of the variables in Y , and fit a simple regression model

$$s = \mu 1 + \beta x + \epsilon. \quad (2)$$

THEOREM 1. *Let V be Pillai's trace statistic for MANOVA of Y on x , and $\hat{\beta}$ be the least-squares estimate of β , then $V = \hat{\beta}$.*

Proof of Theorem 1. Defining $A = (1, Y)$, we have

$$A^T A = \begin{pmatrix} n & 1^T Y \\ Y^T 1 & Y^T Y \end{pmatrix}.$$

Then the inverse of $A^T A$ is

$$(A^T A)^{-1} = \begin{pmatrix} F_{11} & -F_{11} 1^T Y (Y^T Y)^{-1} \\ -\frac{1}{n} F_{22} Y^T 1 & F_{22} \end{pmatrix},$$

where $F_{11} = \{n - 1^T Y (Y^T Y)^{-1} Y^T 1\}^{-1}$ and $F_{22} = (Y^T Y - Y^T 1 1^T Y / n)^{-1}$.
Thus

$$\begin{pmatrix} \hat{a} \\ \hat{b} \end{pmatrix} = (A^T A)^{-1} A^T x = \begin{pmatrix} F_{11} 1^T x - F_{11} 1^T Y (Y^T Y)^{-1} Y^T x \\ -\frac{1}{n} F_{22} Y^T 1 1^T x + F_{22} Y^T x \end{pmatrix},$$

and

$$s = Y\hat{b} = -\frac{1}{n} Y F_{22} Y^T 1 1^T x + Y F_{22} Y^T x.$$

Let $B = (1, x)$, so that

$$B^T B = \begin{pmatrix} n & 1^T x \\ x^T 1 & x^T x \end{pmatrix},$$

$$\det(B^T B) = n x^T x - x^T 1 1^T x, \quad (3)$$

$$(B^T B)^{-1} B^T = \frac{1}{\det(B^T B)} \begin{pmatrix} x^T x 1^T - x^T 1 x^T \\ -1^T x 1^T + n x^T \end{pmatrix}.$$

20 Therefore

$$\begin{aligned} \hat{\beta} &= (0, 1) (B^T B)^{-1} B^T s \\ &= \frac{1}{\det(B^T B)} (-1^T x 1^T + n x^T) \left(-\frac{1}{n} Y F_{22} Y^T 1 1^T x + Y F_{22} Y^T x \right). \end{aligned}$$

By definition, Pillai's trace $V = \text{tr}\{(T - E) T^{-1}\}$, where

$$\begin{aligned} E &= Y^T \left\{ I - B (B^T B)^{-1} B^T \right\} Y, \\ T &= Y^T \left(I - \frac{1}{n} 1 1^T \right) Y. \end{aligned} \tag{4}$$

25

Hence

$$T - E = Y^T \left\{ B (B^T B)^{-1} B^T - \frac{1}{n} 1 1^T \right\} Y. \tag{5}$$

Notice in (4), $T^{-1} = F_{22}$, so combining with (3) and (5), we get

$$\begin{aligned} V &= \text{tr}\{(T - E) T^{-1}\} \\ &= \text{tr}\left\{ Y^T \left(B (B^T B)^{-1} B^T - \frac{1}{n} 1 1^T \right) Y F_{22} \right\} \\ &= \text{tr}\left\{ \left(B (B^T B)^{-1} B^T - \frac{1}{n} 1 1^T \right) Y F_{22} Y^T \right\} \\ &= \text{tr}\left\{ \left(\frac{1}{\det(B^T B)} (1 x^T x 1^T - 1 1^T x x^T) - \frac{1}{n} 1 1^T \right) Y F_{22} Y^T \right\} \\ &\quad + \text{tr}\left\{ \frac{1}{\det(B^T B)} (-x 1^T x 1^T + n x x^T) Y F_{22} Y^T \right\} \\ &= \text{tr}\left\{ \frac{1}{\det(B^T B)} \left(1 x^T x 1^T - \frac{1}{n} 1 \det(B^T B) 1^T - 1 1^T x x^T \right) Y F_{22} Y^T \right\} \\ &\quad + \text{tr}\left\{ \frac{1}{\det(B^T B)} (-x 1^T x 1^T + n x x^T) Y F_{22} Y^T \right\} \\ &= \frac{1}{\det(B^T B)} \text{tr}\left\{ \left(\frac{1}{n} 1 1^T x 1^T x 1^T - 1 1^T x x^T \right) Y F_{22} Y^T \right\} \\ &\quad + \frac{1}{\det(B^T B)} \text{tr}\{(-1^T x 1^T + n x^T) Y F_{22} Y^T x\} \\ &= \frac{1}{\det(B^T B)} \text{tr}\left\{ (1^T x 1^T - n x^T) \frac{1}{n} Y F_{22} Y^T 1 1^T x \right\} \\ &\quad + \frac{1}{\det(B^T B)} \text{tr}\{(-1^T x 1^T + n x^T) Y F_{22} Y^T x\} \\ &= \frac{1}{\det(B^T B)} (-1^T x 1^T + n x^T) \left(-\frac{1}{n} Y F_{22} Y^T 1 1^T x + Y F_{22} Y^T x \right) \\ &= \hat{\beta} \end{aligned}$$

□

Given the numerical equivalence of V and $\hat{\beta}$, $\hat{\beta}$ has the same distribution as V . Note that the correlation coefficient between the fitted values and original response of regression (1) is the same as that of regression (2). Assuming each column of Y follows a Gaussian distribution, let R^2 be the coefficient of determination of regressions (1) and (2), then in regression (2), we have

$$R^2 = \hat{\beta} \frac{Cov(x, s)}{V(s)}$$

Since $x = \hat{a}1 + s + \hat{e}$ and $Cov(s, \hat{a}1 + \hat{e}) = 0$, together with Theorem (1),

$$\hat{\beta} = V = R^2$$

The F-statistic of the multiple regression (1) can be expressed as a function of R^2 , i.e.

$$F = \frac{R^2/k}{(1 - R^2)/(n - k - 1)}$$

which is the same formula for the F-statistic of Pillai's trace V [Pillai, 1960]. After rearranging,

$$\hat{\beta} = V = R^2 = \frac{kF}{(n - k - 1) + kF}$$

As $F \sim F(k, n - k - 1)$, we have

$$\hat{\beta} = V = R^2 \sim Beta\left(\frac{k}{2}, \frac{n - k - 1}{2}\right)$$

which is the exact distribution of $\hat{\beta}$. In practice, the standard error of $\hat{\beta}$ can be obtained by Gaussian approximation of the Beta distribution, which simplifies the significance test of $\hat{\beta}$ as a Wald test.

$\hat{\beta}$ is therefore a simple linear regression effect for a multivariate analysis. This single effect $\hat{\beta}$ is particularly useful in multivariate biological studies, so that the biomarker effect can be interpreted and replicated with meaning, i.e. the effect on the score s .

AUTHOR CONTRIBUTIONS

X.S. initiated and coordinated the study. Z.N. and X.S. proved the theorems. X.S., Z.N. and Y.P. wrote the manuscript and approved the final version.

REFERENCES

- K. C. S. Pillai. Some new test criteria in multivariate analysis. *Ann. Math. Statist.*, 26:117–121, 1955.
 K. C. S. Pillai. *Statistical tables for tests of multivariate hypothesis*. Manila: Statistical Center, University of the Philippines, 1960.